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Searches for lepton-flavour-violating decays of the Higgs boson in $\sqrt{s} = 13$ TeV pp collisions with the ATLAS detector

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ABSTRACT

This Letter presents direct searches for lepton flavour violation in Higgs boson decays, $H \to e\tau$ and $H \to \mu\tau$, performed with the ATLAS detector at the LHC. The searches are based on a data sample of proton–proton collisions at a centre-of-mass energy $\sqrt{s} = 13$ TeV, corresponding to an integrated luminosity of 36.1 fb^{-1}. No significant excess is observed above the expected background from Standard Model processes. The observed (median expected) 95% confidence-level upper limits on the lepton-flavour-violating branching ratios are 0.47% ($0.34^{+0.13}_{-0.10}$%) and 0.28% ($0.37^{+0.14}_{-0.10}$%) for $H \to e\tau$ and $H \to \mu\tau$, respectively.

1. Introduction

The search for processes beyond the Standard Model (SM) is one of the main goals of the Large Hadron Collider (LHC) programme at CERN. A possible sign of such processes is lepton flavour violation (LFV) in decays of the Higgs boson [1,2]. Many beyond-SM theories predict LFV decays of the Higgs boson, such as supersymmetry [3,4], other models with more than one Higgs doublet [5,6], composite Higgs models [7], models with flavour symmetries [8] or warped extra dimensions [9–11] models and others [12,13].

In this Letter, searches for LFV decays of the Higgs boson, $H \to e\tau$ and $H \to \mu\tau$, at the LHC with the ATLAS experiment are presented. Studies are based on proton–proton (pp) collision data recorded in 2015–2016 at a centre-of-mass energy $\sqrt{s} = 13$ TeV. The dataset corresponds to an integrated luminosity of 36.1 fb^{-1}.

Previous ATLAS searches [14,15] placed an upper limit of 1.04% (1.43%) on the $H \to e\tau$ ($H \to \mu\tau$) branching ratio ($\mathcal{B}$) with a 95% confidence level (CL) using Run 1 data collected at $\sqrt{s} = 8$ TeV, corresponding to an integrated luminosity of 20.3 fb^{-1}. The CMS Collaboration recently provided 95% CL upper limits on these branching ratios of 0.61% and 0.25%, respectively, using data collected at $\sqrt{s} = 13$ TeV, with an integrated luminosity of 35.9 fb^{-1} [16].

The searches presented here involve both leptonic ($\tau \to \ell' \nu \bar{\nu}$[1]) and hadronic ($\tau \to$ hadrons $+ \nu$) decays of τ-leptons, denoted $\tau_{\ell'}$ and τ_{had} respectively. The dilepton final state $\ell\tau_{\ell'}$ only considers pairs of different-flavour leptons. Same-flavour lepton pairs are rejected due to the large lepton pair-production Drell-Yan background. Two channels are considered for each of the two searches: $e\tau_\mu$ and $e\tau_{\text{had}}$ for the $H \to e\tau$ search, $\mu\tau_e$ and $\mu\tau_{\text{had}}$ for the $H \to \mu\tau$ search. The analysis is designed such that any potential LFV signal overlap between the $H \to e\tau$ and $H \to \mu\tau$ searches is negligible. Many methods are reused from the measurement of the Higgs boson cross-section in the $H \to \tau\tau$ final state [17].

The ATLAS detector[2] is described in Refs. [18–20]. It consists of an inner tracking detector covering the range $|\eta| < 2.5$, surrounded by a superconducting solenoid providing a 2 T axial magnetic field, high-granularity electromagnetic ($|\eta| < 3.2$) and hadronic calorimeters ($|\eta| < 4.9$), and a muon spectrometer (MS) which covers the range $|\eta| < 2.7$ and includes fast trigger chambers ($|\eta| < 2.4$) and superconducting toroidal magnets.

2. Simulation samples

Samples of Monte Carlo (MC) simulated events are used to optimize the event selection, and to model the signal and several of the background processes. The samples were produced with the ATLAS simulation infrastructure [21] using the full detector simulation performed by the GEANT4 [22] toolkit. The Higgs boson mass was set to $m_H = 125$ GeV [23]. The four leading Higgs boson production mechanisms are considered: the gluon–gluon fusion (ggF), vector-boson fusion (VBF) and two associated production modes

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[1] Unless explicitly mentioned otherwise, leptons (denoted by ℓ or ℓ') refer to electrons or muons.

[2] ATLAS uses a right-handed coordinate system with its origin at the nominal interaction point in the centre of the detector and the z-axis along the beam pipe. The azimuthal angle ϕ runs around the beam pipe, the pseudorapidity is defined in terms of the polar angle θ as $\eta \equiv -\ln\tan(\theta/2)$. Angular distance in the η–ϕ space is defined as $\Delta R \equiv \sqrt{(\Delta\eta)^2 + (\Delta\phi)^2}$.

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Table 1
Generators used to describe the signal and background processes, parton distribution function (PDF) sets for the hard process, and models used for parton showering, hadronization and the underlying event (UEPS). The orders of the total cross-sections used to normalize the events are also given. More details are given in Ref. [17].

Process	Generator	PDF	UEPS	Cross-section order
ggF	Powheg-Box v2 [26–30] NNLOPS [31]	PDF4LHC15 [32] NNLO	Pythia 8.212 [25]	N^3LO QCD + NLO EW [33–36]
VBF	Powheg-Box v2 MiNLO [30]	PDF4LHC15 NLO	Pythia 8.212	∼NNLO QCD + NLO EW [37–39]
WH, ZH	Powheg-Box v2 MiNLO	PDF4LHC15 NLO	Pythia 8.212	NNLO QCD + NLO EW [40–42]
W/Z + jets	Sherpa 2.2.1 [43]	NNPDF30NNLO [44]	Sherpa 2.2.1 [45]	NNLO [46,47]
$VV/V\gamma^*$	Sherpa 2.2.1	NNPDF30NNLO	Sherpa 2.2.1	NNLO
$t\bar{t}$	Powheg-Box v2 [26–28,48]	CT10 [49]	Pythia 6.428 [50]	NNLO+NNLL [51]
Single t	Powheg-Box v1 [52,53]	CT10	Pythia 6.428	NLO [54–56]

(WH, ZH), while the others give negligible contributions and are ignored. The cross-sections of all Higgs boson production processes were normalized to the SM predictions [24]. The LFV Higgs boson decays as well as the $H \to \tau\tau$ and $H \to WW$ background decays were modelled with Pythia 8 [25]. Other background processes involve electroweak production of W/Z bosons via VBF, Drell–Yan production of W/Z in association with jet(s) as well as diboson, single top-quark and top-quark pair ($t\bar{t}$) production. The MC generators used for the SM $H \to \tau\tau$ cross-section measurement [17] were also employed here for all background components. The generators and parton shower models used to simulate different processes are summarized in Table 1.

3. Object reconstruction

The correct identification of $H \to \ell\tau$ events requires reconstruction of several different objects (electrons, muons, and jets, including those initiated by hadronic decays of τ-leptons) and the missing transverse momentum $\vec{p}_{\mathrm{T}}^{\mathrm{miss}}$, whose magnitude is called $E_{\mathrm{T}}^{\mathrm{miss}}$.

Electrons are reconstructed by matching tracks in the inner detector to clustered energy deposits in the electromagnetic calorimeter [57]. Loose likelihood-based identification [58], $p_{\mathrm{T}} > 15$ GeV and fiducial volume requirements ($|\eta| < 2.47$, excluding the transition region between the barrel and the endcap calorimeters $1.37 < |\eta| < 1.52$) are applied. Medium identification, corresponding to an efficiency of 87% at $p_{\mathrm{T}} = 20$ GeV, is imposed for the baseline electron selection.

Muons are identified by tracks reconstructed in the inner detector and matched to tracks in the MS. Loose identification [59], $p_{\mathrm{T}} > 10$ GeV and $|\eta| < 2.5$ requirements are applied. Medium identification (efficiency of 96.1% for muons with $p_{\mathrm{T}} > 20$ GeV) is imposed for the baseline muon selection.

Isolation criteria exploiting calorimeter and track-based information are applied to both electrons and muons. The gradient working point is used, featuring an efficiency of 90% (99%) obtained for leptons with $p_{\mathrm{T}} > 25$ GeV (60 GeV) originating from the $Z \to \ell\ell$ process [58,59].

Jets are reconstructed using the anti-k_t algorithm [60] as implemented by the FastJet [61] package. The algorithm is applied to topological clusters of calorimeter cells [62] with a radius parameter $R = 0.4$. Only jets with $p_{\mathrm{T}} > 20$ GeV and $|\eta| < 4.5$ are considered. Jets from other pp interactions in the same and neighbouring bunch crossings (pile-up) are suppressed using jet vertex tagger (JVT) algorithms [63,64]. Jets containing b-hadrons (b-jets) are identified by the MV2c20 algorithm [65,66] in the central region ($|\eta| < 2.4$). A working point corresponding to 85% average efficiency determined for b-jets in $t\bar{t}$ simulated events is chosen, rejection factors are 2.8 and 28 against c-jets and light-flavour jets respectively.

The reconstruction of the object formed by the visible products of the τ_{had} decay ($\tau_{\mathrm{had\text{-}vis}}$) begins from jets reconstructed by the anti-k_t jet algorithm with a radius parameter $R = 0.4$. Information from the inner detector tracks associated with the energy deposits in the calorimeter is incorporated in the reconstruction. Only $\tau_{\mathrm{had\text{-}vis}}$ candidates with $p_{\mathrm{T}} > 20$ GeV and $|\eta| < 2.5$ are considered.[3] One or three associated tracks with an absolute total charge $|q| = 1$ are required. An identification algorithm [67,68] based on boosted decision trees (BDT) [69–71] is used to reject $\tau_{\mathrm{had\text{-}vis}}$ candidates arising from misidentification of jets or from decays of hadrons with b- or c-quark content. Unless otherwise indicated, a tight identification (ID) working point is used for the $\tau_{\mathrm{had\text{-}vis}}$, corresponding to an efficiency of 60% (45%) for 1-prong (3-prong) candidates. Jets corresponding to identified $\tau_{\mathrm{had\text{-}vis}}$ candidates are removed from the jet collection. The $\tau_{\mathrm{had\text{-}vis}}$ candidates with one track overlapping with an electron candidate with high ID score, as determined by a multivariate (MVA) approach, are rejected. Leptonic τ-decays are reconstructed as electrons or muons.

Events considered in the analysis are triggered with single-electron or single-muon triggers. The p_{T} thresholds depend on the isolation requirement and data-taking period [72,73]. The lowest trigger thresholds correspond to $25 - 27$ GeV (electrons) and $21 - 27$ GeV (muons).

4. Event selection and categorization

Events selected in the $\ell\tau_{\ell'}$ channel contain exactly one electron and one muon of opposite-sign (OS) charges. Similarly in the $\ell\tau_{\mathrm{had}}$ channel, a lepton and a $\tau_{\mathrm{had\text{-}vis}}$ of OS charges are required, and events with more than one baseline lepton are rejected. The selection criteria are summarized in Table 2 for the analysis categories as well as the control regions (CRs), which are described in Section 5.

In the $\ell\tau_{\ell'}$ channel, ℓ_1 and ℓ_2 denote the leading and subleading lepton in p_{T}, respectively. Events where the leading lepton is an electron (muon) are used in the search for $H \to e\tau_\mu$ ($H \to \mu\tau_e$). A requirement on the dilepton invariant mass, equal to the invariant mass of the lepton and the visible τ-decay products, m_{vis}, reduces backgrounds with top quarks, and the criterion applied to the track-to-cluster p_{T} ratio of the electron reduces the $Z \to \mu\mu$ background where a muon deposits a large amount of energy in the electromagnetic calorimeter and is misidentified as an electron in the $\mu\tau_e$ channel. The contribution from the $H \to \tau\tau$ decay is reduced by the asymmetric p_{T} selection of the two leptons.

In the $\ell\tau_{\mathrm{had}}$ channel, the criterion based on the azimuthal separations of lepton–$E_{\mathrm{T}}^{\mathrm{miss}}$ and $\tau_{\mathrm{had\text{-}vis}}$–$E_{\mathrm{T}}^{\mathrm{miss}}$, $\sum_{i=\ell,\tau_{\mathrm{had\text{-}vis}}} \cos\Delta\phi(i, E_{\mathrm{T}}^{\mathrm{miss}})$, reduces the W + jets background whereas the requirement on $|\Delta\eta(\ell, \tau_{\mathrm{had\text{-}vis}})|$ reduces backgrounds with misidentified $\tau_{\mathrm{had\text{-}vis}}$ candidates.

For both channels of each search, a b-veto requirement reduces the single-top-quark and $t\bar{t}$ backgrounds. Events are further cate-

[3] The transition region in η is excluded, similarly to electrons.

Table 2
Baseline event selection and further categorization for the $\ell\tau_{\ell'}$ and $\ell\tau_{\text{had}}$ channels. The same criteria are also used for the control region (CR) definitions in the $\ell\tau_{\ell'}$ channel (Section 5), but one requirement of the baseline selection is inverted to achieve orthogonal event selection. There is no CR in the $\ell\tau_{\text{had}}$ channel.

Selection	$\ell\tau_{\ell'}$	$\ell\tau_{\text{had}}$
Baseline	exactly 1e and 1μ, OS $p_{\text{T}}^{\ell_1} > 45$ GeV $p_{\text{T}}^{\ell_2} > 15$ GeV 30 GeV $< m_{\text{vis}} <$ 150 GeV $p_{\text{T}}^{e}(\text{track})/p_{\text{T}}^{e}(\text{cluster}) < 1.2$ ($\mu\tau_e$ only)	exactly 1ℓ and 1$\tau_{\text{had-vis}}$, OS $p_{\text{T}}^{\ell} > 27.3$ GeV $p_{\text{T}}^{\tau_{\text{had-vis}}} > 25$ GeV, $\lvert\eta^{\tau_{\text{had-vis}}}\rvert < 2.4$ $\sum_{i=\ell,\tau_{\text{had-vis}}} \cos\Delta\phi(i, E_{\text{T}}^{\text{miss}}) > -0.35$ $\lvert\Delta\eta(\ell, \tau_{\text{had-vis}})\rvert < 2$
	b-veto (for jets with $p_{\text{T}} > 25$ GeV and $\lvert\eta\rvert < 2.4$)	b-veto (for jets with $p_{\text{T}} > 25$ GeV and $\lvert\eta\rvert < 2.4$)
VBF	Baseline ≥ 2 jets, $p_{\text{T}}^{\text{j}_1} > 40$ GeV, $p_{\text{T}}^{\text{j}_2} > 30$ GeV $\lvert\Delta\eta(\text{j}_1, \text{j}_2)\rvert > 3$, $m(\text{j}_1, \text{j}_2) > 400$ GeV –	Baseline ≥ 2 jets, $p_{\text{T}}^{\text{j}_1} > 40$ GeV, $p_{\text{T}}^{\text{j}_2} > 30$ GeV $\lvert\Delta\eta(\text{j}_1, \text{j}_2)\rvert > 3$, $m(\text{j}_1, \text{j}_2) > 400$ GeV $p_{\text{T}}^{\tau_{\text{had-vis}}} > 45$ GeV
Non-VBF	Baseline plus fail VBF categorization $m_{\text{T}}(\ell_1, E_{\text{T}}^{\text{miss}}) > 50$ GeV $m_{\text{T}}(\ell_2, E_{\text{T}}^{\text{miss}}) < 40$ GeV $\lvert\Delta\phi(\ell_2, E_{\text{T}}^{\text{miss}})\rvert < 1.0$ $p_{\text{T}}^{\tau}/p_{\text{T}}^{\ell_1} > 0.5$	Baseline plus fail VBF categorization – – – –
Top-quark CR VBF and non-VBF	inverted b-veto: ≥ 1 b-tagged jet ($p_{\text{T}} > 25$ GeV and $\lvert\eta\rvert < 2.4$)	
$Z \to \tau\tau$ CR VBF and non-VBF	inverted $p_{\text{T}}^{\ell_1}$ requirement: 35 GeV $< p_{\text{T}}^{\ell_1} <$ 45 GeV	

gorized into VBF (with a focus on the VBF production of the Higgs boson) and non-VBF categories. The VBF selection is based on the kinematics of the two jets with the highest p_{T}, where j_1 and j_2 denote the leading and subleading jet in p_{T}, respectively. The variables $m(\text{j}_1, \text{j}_2)$ and $\Delta\eta(\text{j}_1, \text{j}_2)$ stand for the invariant mass and η separation of these two jets. The non-VBF category contains events failing the VBF selection. In the dilepton channel, additional selection criteria are applied to further reject background events in this category. These criteria are also listed in Table 2, where m_{T} stands for the transverse mass[4] of the two objects listed in parentheses, and p_{T}^{τ} represents the magnitude of the vector sum of $p_{\text{T}}^{\ell_2}$ and $E_{\text{T}}^{\text{miss}}$. The requirement on $p_{\text{T}}^{\tau}/p_{\text{T}}^{\ell_1}$ reduces the background arising from jets misidentified as leptons. The VBF and non-VBF categories in each of the $\ell\tau_{\ell'}$ and $\ell\tau_{\text{had}}$ channels give rise to four signal regions in each search.

The analysis exploits BDT algorithms to enhance the signal separation from the background in the individual searches, channels and categories. The components of the four-momenta of the analysis objects as well as derived event variables (e.g. invariant masses and angular separations) are the input variables of the BDT discriminant. Correlations between these input variables have been carefully checked, highly correlated variables have been removed and the remaining ones are ranked according to their discrimination power [74,75]. The list of variables is then optimized, removing the lowest-ranked variables with marginal contribution to the sensitivity. The final list of variables is presented in Table 3 for each channel and category. The invariant mass of the Higgs boson reconstructed under the $H \to \ell\tau$ decay hypothesis exhibits the highest signal-to-background separation power and it helps to distinguish LFV signal from $H \to \tau\tau$ and $H \to WW$ backgrounds. For the $\ell\tau_{\ell'}$ channel the invariant mass is reconstructed with the MMC algorithm [76] and is denoted by m_{MMC}; for the $\ell\tau_{\text{had}}$ channel it is reconstructed with the collinear approximation [76] and is denoted by m_{coll}. The analysis CRs are used to validate the level of agreement between data and simulated distributions of the BDT score and input variables, as well as their correlations.

5. Background modelling

The most significant backgrounds in the search are from events with $Z \to \tau\tau$ decays or with (single or pair-produced) top quarks, especially in the $\ell\tau_{\ell'}$ channel, as well as from events with misidentified objects, which are estimated using data-driven (d.d.) techniques. The relative contribution from misidentified objects to the total background yield is 5–25% in the $\ell\tau_{\ell'}$ channel and 25–45% in the $\ell\tau_{\text{had}}$ channel, depending on the search and the analysis category. The shapes of distributions from the $Z \to \tau\tau$ and top-quark (single-top-quark and $t\bar{t}$) processes are modelled by simulation in both the $\ell\tau_{\ell'}$ and $\ell\tau_{\text{had}}$ decay channels. In the $\ell\tau_{\ell'}$ channel, the relative contributions of $Z \to \tau\tau$ and top-quark production processes are 20–35% and 20–55%, respectively; the top-quark background dominates in the VBF category. In the $\ell\tau_{\text{had}}$ channel, the top-quark background fraction is 1–10%, while the $Z \to \tau\tau$ process contributes to 45–55% of the total background. The individual contributions are listed in Tables 4 and 5. Smaller background components are also modelled by simulation and are grouped together: $Z \to \mu\mu$, diboson production, $H \to \tau\tau$ and $H \to WW$.

Good modelling of the background is demonstrated in Fig. 1 for a selection of important BDT input variables. Details of the background estimation techniques are given below.

5.1. $\ell\tau_{\ell'}$ channel

Two sets of CRs, as defined in Table 2, are used to constrain the normalization of $Z \to \tau\tau$ and top-quark background components. These CRs inherit their definitions from the corresponding analysis category but invert one requirement to ensure orthogonality with the nominal selection. The normalization factors are determined during the statistical analysis by fitting the event yields in all signal and control regions simultaneously. For each search, separate $Z \to \tau\tau$ normalization factors are used for the VBF and non-VBF categories. In the case of the top-quark background, in

[4] The transverse mass of two objects is defined as $m_{\text{T}} = \sqrt{2 p_{\text{T}1} p_{\text{T}2}(1 - \cos\Delta\phi)}$, where $p_{\text{T}i}$ are the individual transverse momenta and $\Delta\phi$ is the angle between the two objects in the azimuthal plane.

Table 3
BDT input variables used in the analysis. For each channel and category, used input variables are marked with HR (indicating the five variables with the highest rank) or a bullet. Analogous variables between the two channels are listed on the same line.

$\ell\tau_{\ell'}$			$\ell\tau_{\mathrm{had}}$		
Variable	VBF	non-VBF	Variable	VBF	non-VBF
m_{MMC}	HR	HR	m_{coll}	HR	HR
$p_{\mathrm{T}}^{\ell_1}$	•	•	p_{T}^{ℓ}	•	HR
$p_{\mathrm{T}}^{\ell_2}$	HR	HR	$p_{\mathrm{T}}^{\tau_{\text{had-vis}}}$	•	HR
$\Delta R(\ell_1, \ell_2)$	HR	•	$\Delta R(\ell, \tau_{\text{had-vis}})$	•	•
$m_{\mathrm{T}}(\ell_1, E_{\mathrm{T}}^{\mathrm{miss}})$	•	HR	$m_{\mathrm{T}}(\ell, E_{\mathrm{T}}^{\mathrm{miss}})$	HR	•
$m_{\mathrm{T}}(\ell_2, E_{\mathrm{T}}^{\mathrm{miss}})$	HR	•	$m_{\mathrm{T}}(\tau_{\text{had-vis}}, E_{\mathrm{T}}^{\mathrm{miss}})$	HR	HR
$\Delta\phi(\ell_1, E_{\mathrm{T}}^{\mathrm{miss}})$	•	•	$\Delta\phi(\ell, E_{\mathrm{T}}^{\mathrm{miss}})$	HR	•
$\Delta\phi(\ell_2, E_{\mathrm{T}}^{\mathrm{miss}})$		HR	$\Delta\phi(\tau_{\text{had-vis}}, E_{\mathrm{T}}^{\mathrm{miss}})$	•	
$m(\mathrm{j}_1, \mathrm{j}_2)$	•		$m(\mathrm{j}_1, \mathrm{j}_2)$	•	
$\Delta\eta(\mathrm{j}_1, \mathrm{j}_2)$	HR		$\Delta\eta(\mathrm{j}_1, \mathrm{j}_2)$	•	
$p_{\mathrm{T}}^{\tau}/p_{\mathrm{T}}^{\ell_1}$		HR	$\sum_{i=\ell,\tau_{\text{had-vis}}} \cos\Delta\phi(i, E_{\mathrm{T}}^{\mathrm{miss}})$	•	•
			$E_{\mathrm{T}}^{\mathrm{miss}}$	HR	•
			m_{vis}		HR
			$\Delta\eta(\ell, \tau_{\text{had-vis}})$		•
			η^{ℓ}		•
			$\eta^{\tau_{\text{had-vis}}}$		•
			ϕ^{ℓ}		•
			$\phi^{\tau_{\text{had-vis}}}$		•
			$\phi(E_{\mathrm{T}}^{\mathrm{miss}})$		•

Table 4
Event yields and predictions as determined by the background-only fit in different signal regions of the $H \to e\tau$ analysis. Uncertainties include both the statistical and systematic contributions. "Other" contains diboson, $Z \to \ell\ell$, $H \to \tau\tau$ and $H \to WW$ background processes. For the $e\tau_{\mathrm{had}}$ channel the "$Z \to ee$ (d.d.)" component corresponds to electrons misidentified as $\tau_{\text{had-vis}}$. This contribution is summed with "Other" since there are few events in the VBF category. The uncertainty of the total background includes all correlations between channels. The normalizations of top-quark ($\ell\tau_{\ell'}$ channel only) and $Z \to \tau\tau$ background components are determined by the fit, while the expected signal event yields are given for $\mathcal{B}(H \to e\tau) = 1\%$.

	$e\tau_{\mu}$ non-VBF	$e\tau_{\mu}$ VBF	$e\tau_{\mathrm{had}}$ non-VBF	$e\tau_{\mathrm{had}}$ VBF
Signal	379 ± 31	19.8 ± 2.7	1180 ± 110	25 ± 4
$Z \to \tau\tau$	2470 ± 230	221 ± 34	73 800 ± 1900	290 ± 40
Top-quark	1640 ± 140	490 ± 40	1580 ± 190	56 ± 12
Mis-identified	1330 ± 250	73 ± 33	74 400 ± 1600	140 ± 50
$Z \to ee$ (d.d.)			15 900 ± 1800	82 ± 13
Other	1700 ± 80	220 ± 15	2960 ± 200	
Total background	7130 ± 100	1003 ± 33	168 700 ± 1000	570 ± 40
Data	7128	992	168 883	572

Table 5
Event yields and predictions as determined by the background-only fit in different signal regions of the $H \to \mu\tau$ analysis. Uncertainties include both the statistical and systematic contributions. "Other" contains diboson, $Z \to \ell\ell$, $H \to \tau\tau$ and $H \to WW$ background processes. The uncertainty of the total background includes all correlations between channels. The normalizations of top-quark ($\ell\tau_{\ell'}$ channel only) and $Z \to \tau\tau$ background components are determined by the fit, while the expected signal event yields are given for $\mathcal{B}(H \to \mu\tau) = 1\%$.

	$\mu\tau_{e}$ non-VBF	$\mu\tau_{e}$ VBF	$\mu\tau_{\mathrm{had}}$ non-VBF	$\mu\tau_{\mathrm{had}}$ VBF
Signal	287 ± 23	14.6 ± 1.9	1200 ± 120	25 ± 5
$Z \to \tau\tau$	1860 ± 130	144 ± 26	96 100 ± 2000	274 ± 33
Top quark	1260 ± 130	390 ± 34	1620 ± 210	51 ± 10
Misidentified	1340 ± 210	41 ± 21	63 900 ± 1600	149 ± 33
Other	1180 ± 140	168 ± 18	23 000 ± 1000	104 ± 15
Total background	5640 ± 100	743 ± 29	184 500 ± 1200	580 ± 30
Data	5664	723	184 508	583

which leading jets are produced at a lower order of the perturbative expansion of the scattering process, a combined normalization factor across the two categories is used in the $\ell\tau_{\ell'}$ channel.

Top-quark CRs are almost exclusively composed of top-quark backgrounds: the purity is 95% across both searches and categories, with $t\bar{t}$ process accounting for more than 90% of the top-quark backgrounds. The $Z \to \tau\tau$ CRs achieved a purity of ~80% in the non-VBF categories, while a lower purity of ~60% is observed in the VBF categories. The contributions of all other background components are normalized to their SM predictions when the likelihood fit (Section 7) is applied.

The shape and normalization of diboson and $Z \to \mu\mu$ background distributions are validated with data in dedicated regions where their contributions are enhanced. The latter process only contributes sizeably in the $\mu\tau_e$ channel, where it represents up to 10% of the total background.

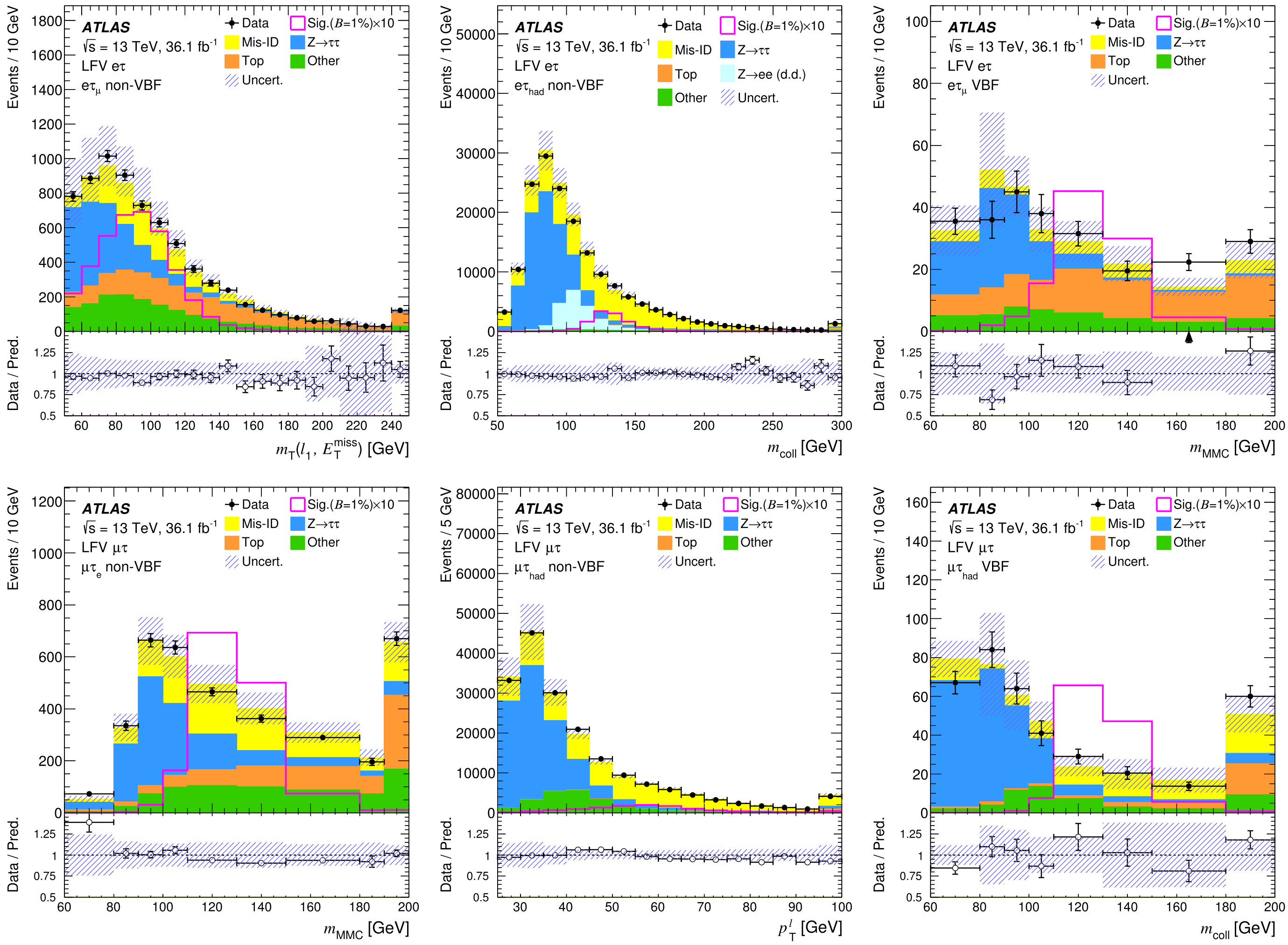

Fig. 1. Distributions of representative kinematic quantities for different searches, channels and categories, before the fit as described in Section 7 is applied. Top row: transverse mass $m_T(\ell_1, E_T^{miss})$ ($e\tau_\mu$ non-VBF), collinear mass m_{coll} ($e\tau_{had}$ non-VBF) and m_{MMC} ($e\tau_\mu$ VBF). Bottom row: m_{MMC} ($\mu\tau_e$ non-VBF), muon p_T ($\mu\tau_{had}$ non-VBF) and m_{coll} ($\mu\tau_{had}$ VBF). Entries with values that would exceed the x-axis range are included in the last bin of each distribution. The size of the combined statistical, experimental and theoretical uncertainties in the background is indicated by the hatched bands. The $H \to e\tau$ ($H \to \mu\tau$) signal overlaid in top (bottom) plots assumes $\mathcal{B}(H \to \ell\tau) = 1\%$ and is enhanced by a factor 10. In the data/background prediction ratio plots, points outside the displayed y-axis range are shown by arrows.

Another source of background comes from $W+$jets, top-quark and multi-jet events, where jets are misidentified as leptons. This background is estimated directly from OS data events where an inverted isolation requirement is imposed on the subleading lepton [17]. Normalization factors are applied to correct for the inverted isolation requirement. The normalization factors are derived in a dedicated region where the leptons are required to have same-sign (SS) charges. Additional corrections are made by reweighting the MC distributions of $\Delta\phi(\ell_1, E_T^{miss})$ and $\Delta\phi(\ell_2, E_T^{miss})$ to data in the SS region, which improves the modelling of azimuthal angles between leptons and the E_T^{miss} direction as well as the modelling of $m_T(\ell_2, E_T^{miss})$. A similar improvement is observed in the nominal OS region. In most of the cases, the misidentified jet mimics the lepton of lower p_T, ℓ_2, while the fraction of events where both leptons are misidentified varies between 2% to 8% across categories. The systematic uncertainties of the estimation of the misidentified lepton background include contributions from closure tests in SS and OS regions enriched with misidentified leptons, from the corrections made to the $\Delta\phi$ distributions, and from the composition of the misidentified lepton background.

5.2. $\ell\tau_{had}$ channel

The main background contributions come from the $Z \to \tau\tau$ process and events where either a jet or an electron is misidentified as $\tau_{had\text{-}vis}$. The shape of the $Z \to \tau\tau$ background distribution is modelled by simulation, and the corresponding normalization factors are determined from the simultaneous fit of the event yields in all signal and control regions. The $Z \to \tau\tau$ normalization factors are fully correlated with those of the $\ell\tau_{\ell'}$ channel, in each VBF and non-VBF category. Top-quark production represents less than 1% of the total background in the $\ell\tau_{had}$ channel and is determined by simulation, including its normalization, which is kept fixed in the fit.

The main contributions to jets misidentified as $\tau_{had\text{-}vis}$ come from multi-jet events and W-boson production in association with jets, and a fake-factor method is used to estimate the contribution of each component separately. A fake factor is defined as the ratio of the number of events where the highest-p_T jet is identified as a tight $\tau_{had\text{-}vis}$ candidate to the number of events where the highest-p_T jet fails to satisfy this τ-ID criterion but satisfies a looser criterion. The procedure, including systematic uncertainties, is described in Ref. [17]. Since a different τ-ID working point is considered in this analysis, fake factors are re-derived as a function of p_{T} and track multiplicity of the $\tau_{\text{had-vis}}$ candidate.

Electrons misidentified as $\tau_{\text{had-vis}}$, denoted by "$Z \to ee$ (d.d.)" in the following figures and tables, represent another background component in the $e\tau_{\text{had}}$ channel, with a contribution about five times smaller than that of jets misidentified as $\tau_{\text{had-vis}}$. While the rate of electrons misidentified as 3-prong $\tau_{\text{had-vis}}$ makes a negligible contribution and is modelled by simulation, the rate of electrons misidentified as 1-prong $\tau_{\text{had-vis}}$ is determined with a fake-factor method. This time, the fake factor is defined as the ratio of the number of events with tight τ-ID to the number of events with anti-identified $\tau_{\text{had-vis}}$ (such a candidate satisfies all criteria but the requirement on the high electron ID score is inverted). These fake factors are derived in a dedicated $Z \to ee$ enriched region defined by $|m_{\text{vis}} - m_Z| < 5$ GeV, $m_{\mathrm{T}}(\ell, E_{\mathrm{T}}^{\text{miss}}) < 40$ GeV, and $m_{\mathrm{T}}(\tau_{\text{had-vis}}, E_{\mathrm{T}}^{\text{miss}}) < 60$ GeV, where the $\tau_{\text{had-vis}}$ candidate satisfies the medium τ-ID (corresponding to an efficiency of 55% and 40% for 1-prong and 3-prong candidates, respectively) but not the tight τ-ID criterion to avoid overlap with the $\ell\tau_{\text{had}}$ signal region. These fake factors are applied to signal-like events with the anti-identified $\tau_{\text{had-vis}}$ to determine the background contribution in the categories of the analysis. The systematic uncertainties include the statistical uncertainty of the fake factors and account for looser τ-ID in the $Z \to ee$ enriched region as well as for the subtraction of the not misidentified components in this region.

6. Systematic uncertainties

The systematic uncertainties affect the normalization of signal and background, and/or the shape of their corresponding final discriminant distributions. Each source of systematic uncertainty is considered to be uncorrelated with the other sources. The effect of each systematic uncertainty is fully considered in each category, including control regions. Correlations of each systematic uncertainty are maintained across processes, channels, categories and regions. The size of the systematic uncertainties and their impact on the fitted branching ratio are discussed in Section 7. The main sources of systematic uncertainties are related to the estimation of the backgrounds originating from mis-identified leptons/jets and to the jet energy scale uncertainties.

Experimental uncertainties include those originating from the reconstruction, identification, tagging and triggering efficiencies of all physics objects as well as their momentum scale and resolution. These include effects from leptons [57–59], $\tau_{\text{had-vis}}$ [68], jets [63,64,77] and $E_{\mathrm{T}}^{\text{miss}}$ [78]. Uncertainties affecting the kinematics of the physics objects are propagated to the BDT input variables. The corresponding shape and normalization variations of the BDT discriminant are considered in the statistical analysis. Uncertainties of the luminosity measurement [79], pile-up modelling and uncertainties specific to mis-identified background estimation techniques mentioned in Section 5 are included.

The procedures to estimate the uncertainty of the Higgs boson production cross-sections follow the recommendations of the LHC Higgs Cross-Section Working Group [80]. Theoretical uncertainties affecting the ggF signal originate from nine sources [24]. Two sources account for yield uncertainties, which are evaluated by an overall variation of all relevant scales and are correlated across all bins of the BDT discriminant distribution [81]. Another two sources account for migration uncertainties of zero to one jet and one to at least two jets in the event [81–83], two for Higgs boson p_{T} shape uncertainties, one for the treatment of the top-quark mass in the loop corrections, and two for the acceptance uncertainties of ggF production in the VBF phase space from selecting exactly two and at least three jets, respectively [84,85]. For VBF and WH, ZH production cross-sections, the uncertainties due to missing higher-order QCD corrections are estimated by varying the factorization and renormalization scales up and down by factors of two around the nominal scale. For all signal samples, PDF uncertainties are estimated using 30 eigenvector variations and two α_{s} variations using the default PDF set PDF4LHC15 [32]. Uncertainties related to the simulation of the underlying event, hadronization and parton shower are estimated by comparing the acceptances when using Pythia 8.212 [25] or Herwig 7.0.3 [86,87].

The sources of modelling uncertainties considered for the $Z \to \tau\tau$ process are the same as in Ref. [17] and their effect on the event migrations between categories and on the shape of the BDT discriminant are considered, since the overall normalizations are determined from data in the statistical analysis. These systematic uncertainties include variations of PDF sets, factorization and renormalization scales, CKKW matching [88], resummation scale and parton shower modelling. The other background processes are either normalized using data (processes with top-quarks and misidentified leptons and $\tau_{\text{had-vis}}$ candidates) or their cross-section uncertainties have negligible impact and therefore are not included. The shape uncertainties of these backgrounds originate from experimental uncertainties only.

7. Statistical analysis

The searches for $H \to e\tau$ and $H \to \mu\tau$ are treated independently. For each search, the analysis exploits the four signal regions and the two control regions specified in Table 2. The BDT score distributions of all signal regions are analysed to test the presence of a signal, simultaneously with the event yields in control regions, which are included to constrain the normalizations of the major backgrounds estimated from simulation. The statistical analysis uses a binned likelihood function $\mathcal{L}(\mu, \theta)$, constructed as a product of Poisson probability terms over all bins considered in the search. This function depends on the parameter μ, defined as the branching ratio $\mathcal{B}(H \to \ell\tau)$, and a set of nuisance parameters θ that encode the effect of systematic uncertainties in the signal and background expectations. All nuisance parameters are implemented in the likelihood function as Gaussian or log-normal constraints. The normalization factors of the single-top-quark and $t\bar{t}$ backgrounds in the $\ell\tau_{\ell'}$ channel and of the $Z \to \tau\tau$ background component are unconstrained parameters of the fit. Estimates of the parameters of interest are calculated with the profile-likelihood-ratio test statistic $\tilde{q}_{\mu}$ [89], and the upper limits on the branching ratios are derived by using $\tilde{q}_{\mu}$ and the $\mathrm{CL_S}$ method [90].

The discriminant distributions after the fit in each channel are shown in Figs. 2 and 3. Good agreement between data and the background expectation is observed. The event yields after the background-only fit are summarized in Tables 4 and 5. In the non-VBF category, the yields in the $\ell\tau_{\text{had}}$ channel are larger than in the $\ell\tau_{\ell'}$ channel due to the looser selection criteria defined for the former channel (Section 4). Table 6 shows a summary of the uncertainties of $\mathcal{B}(H \to \ell\tau)$. The uncertainties associated with misidentified leptons and $\tau_{\text{had-vis}}$ candidated and those related to the jet energy scale and resolution exhibit the highest impact on the best-fit branching ratios in both searches. The combined impact from all systematic uncertainties and the data statistics ranges from 0.17% to 0.19%.

8. Results

The best-fit branching ratios and upper limits are computed while assuming $\mathcal{B}(H \to \mu\tau) = 0$ for the $H \to e\tau$ search and $\mathcal{B}(H \to e\tau) = 0$ for the $H \to \mu\tau$ search. The best-fit values of the LFV Higgs boson branching ratios are equal to $(0.15^{+0.18}_{-0.17})$% and (-0.22 ± 0.19)% for the $H \to e\tau$ and $H \to \mu\tau$ search, respectively.

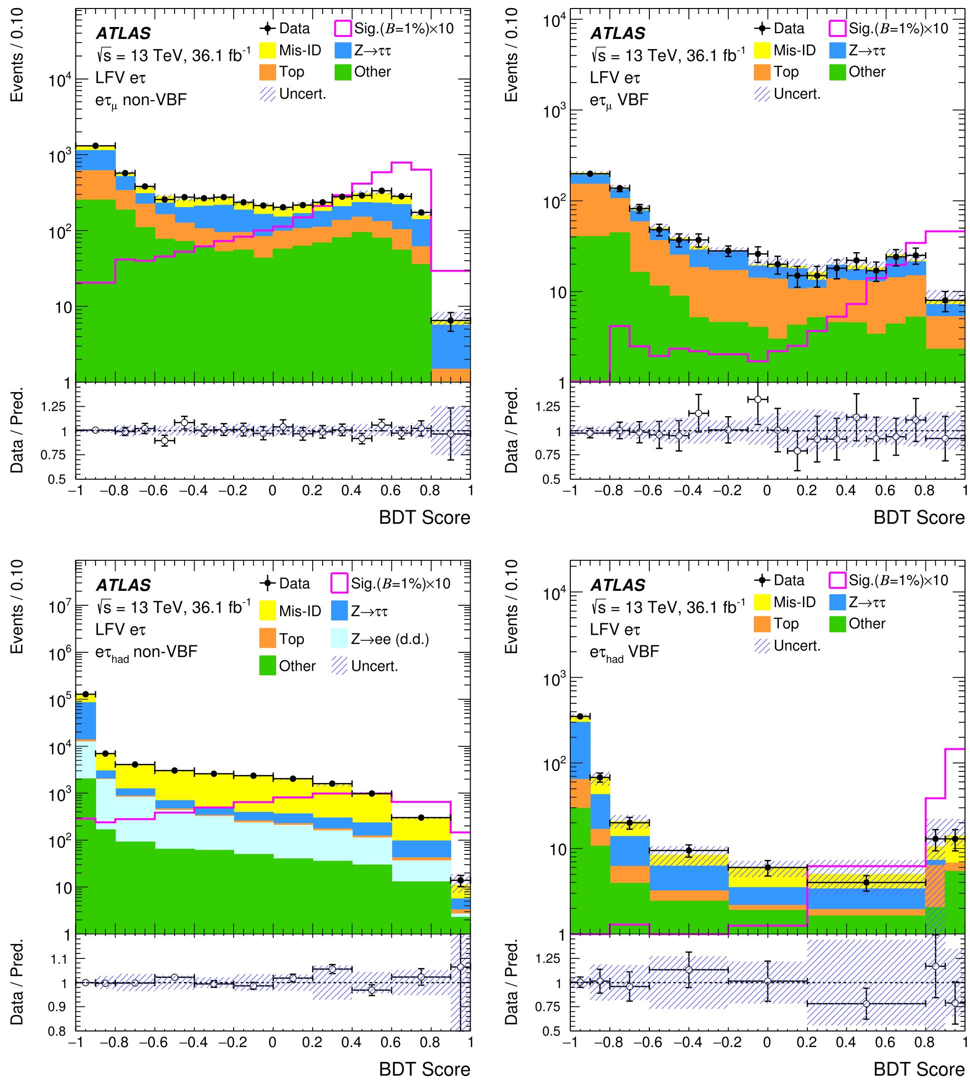

Fig. 2. Distributions of the BDT score after the background+signal fit in each signal region of the $e\tau$ search, with the LFV signal overlaid, normalized with $\mathcal{B}(H \to e\tau) = 1\%$ and enhanced by a factor 10 for visibility. The top and bottom plots display $e\tau_\mu$ and $e\tau_{\text{had}}$ BDT scores respectively, the left (right) column corresponds to the non-VBF (VBF) category. The size of the combined statistical, experimental and theoretical uncertainties of the background is indicated by the hatched bands. The binning is shown as in the statistical analysis.

Table 6
Summary of the systematic uncertainties and their impact on the best-fit value of $\mathcal{B}$ in the $H \to e\tau$ and $H \to \mu\tau$ searches. The measured values are obtained by the fit to data, while the expected values are determined by the fit to a background-only sample.

Source of uncertainty	Impact on $\mathcal{B}(H \to e\tau)$ [%]		Impact on $\mathcal{B}(H \to \mu\tau)$ [%]	
	Measured	Expected	Measured	Expected
Electron	$+0.05/-0.05$	$+0.06/-0.06$	$+0.03/-0.03$	$+0.02/-0.02$
Muon	$+0.04/-0.04$	$+0.04/-0.04$	$+0.10/-0.10$	$+0.08/-0.10$
$\tau_{\text{had-vis}}$	$+0.02/-0.02$	$+0.02/-0.02$	$+0.04/-0.04$	$+0.04/-0.05$
Jet	$+0.09/-0.08$	$+0.09/-0.09$	$+0.11/-0.12$	$+0.11/-0.12$
$E_{\text{T}}^{\text{miss}}$	$+0.02/-0.02$	$+0.02/-0.03$	$+0.05/-0.08$	$+0.03/-0.05$
b-tag	$+0.02/-0.03$	$+0.03/-0.03$	$+0.01/-0.01$	$+0.01/-0.01$
Mis-ID backg. ($\ell\tau_{\ell'}$)	$+0.08/-0.07$	$+0.09/-0.08$	$+0.07/-0.07$	$+0.07/-0.07$
Mis-ID backg. ($\ell\tau_{\text{had}}$)	$+0.12/-0.11$	$+0.11/-0.12$	$+0.11/-0.11$	$+0.10/-0.10$
Pile-up modelling	$+0.02/-0.01$	$+0.01/-0.01$	$+0.05/-0.03$	$+0.08/-0.06$
Luminosity	< 0.01	< 0.01	< 0.01	< 0.01
Background norm.	$+0.05/-0.04$	$+0.05/-0.03$	$+0.04/-0.02$	$+0.05/-0.03$
Theor. uncert. (backg.)	$+0.04/-0.03$	$+0.04/-0.03$	$+0.08/-0.07$	$+0.09/-0.09$
Theor. uncert. (signal)	$+0.01/-0.01$	$+0.01/-0.01$	$+0.04/-0.02$	$+0.02/-0.02$
MC statistics	$+0.04/-0.04$	$+0.03/-0.03$	$+0.04/-0.04$	$+0.05/-0.04$
Full systematic	$+0.17/-0.16$	$+0.17/-0.17$	$+0.18/-0.18$	$+0.19/-0.20$
Data statistics	$+0.07/-0.07$	$+0.07/-0.07$	$+0.07/-0.07$	$+0.08/-0.08$
Total	$+0.18/-0.17$	$+0.18/-0.18$	$+0.19/-0.19$	$+0.20/-0.21$

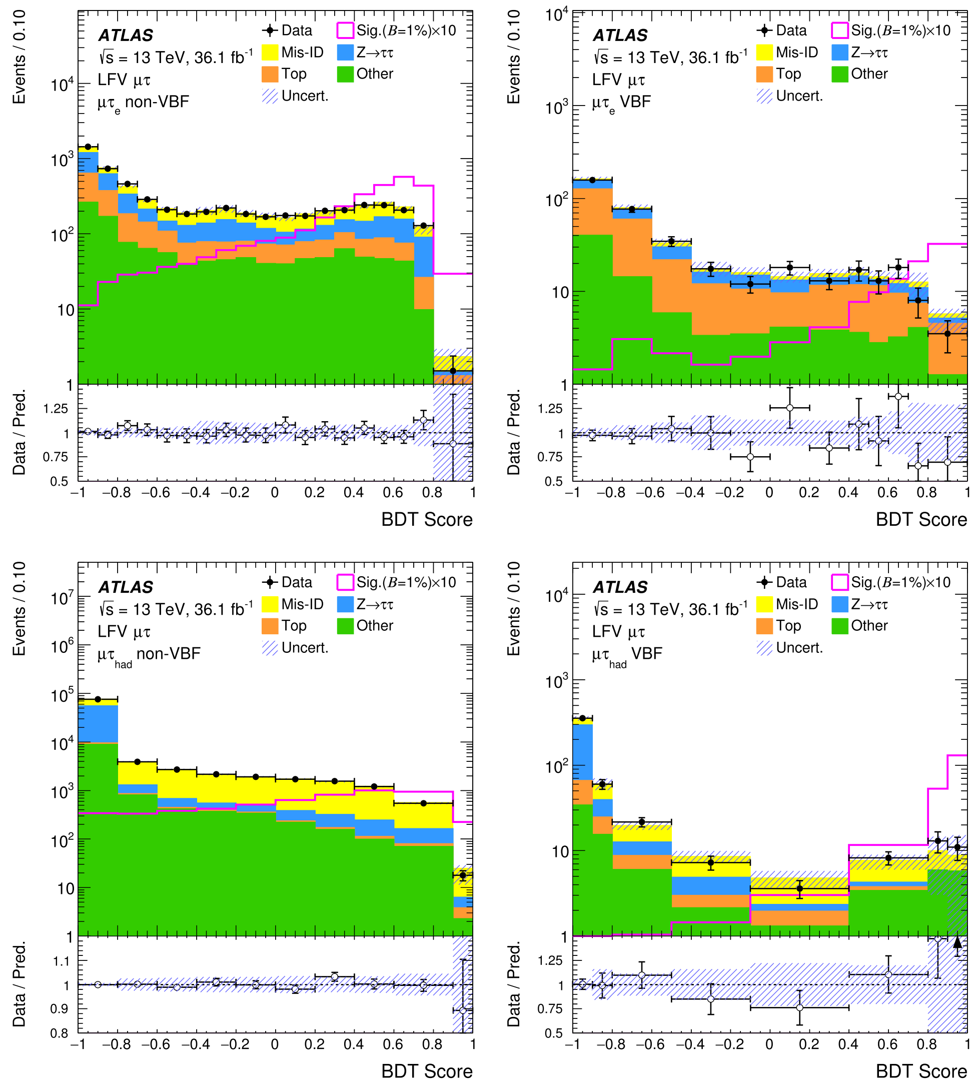

Fig. 3. Distributions of the BDT score after the background+signal fit in each signal region of the $\mu\tau$ search, with the LFV signal overlaid, normalized with $\mathcal{B}(H \to \mu\tau) = 1\%$ and enhanced by a factor 10 for visibility. The top and bottom plots display $\mu\tau_e$ and $\mu\tau_{\text{had}}$ BDT scores respectively, the left (right) column corresponds to the non-VBF (VBF) category. The size of the combined statistical, experimental and theoretical uncertainties of the background is indicated by the hatched bands. The binning is shown as in the statistical analysis. In the data/background prediction ratio plots, points outside the displayed y-axis range are shown by arrows.

In the absence of a significant excess, upper limits on the LFV branching ratios are set for a Higgs boson with $m_H = 125$ GeV. The observed (median expected) 95% CL upper limits are 0.47% ($0.34^{+0.13}_{-0.10}$%) and 0.28% ($0.37^{+0.14}_{-0.10}$%) for the $H \to e\tau$ and $H \to \mu\tau$ searches, respectively. These limits are significantly lower than the corresponding Run 1 limits of Refs. [14,15]. The breakdown of contributions from different signal regions is shown in Fig. 4.

The branching ratio of the LFV Higgs boson decay is related to the non-diagonal Yukawa coupling matrix elements [91] by the formula

$$|Y_{\ell\tau}|^2 + |Y_{\tau\ell}|^2 = \frac{8\pi}{m_H} \frac{\mathcal{B}(H \to \ell\tau)}{1 - \mathcal{B}(H \to \ell\tau)} \Gamma_H(\text{SM}),$$

where $\Gamma_H(\text{SM}) = 4.07$ MeV [92] stands for the Higgs boson width as predicted by the Standard Model. Thus, the observed limits on the branching ratio correspond to the following limits on the coupling matrix elements: $\sqrt{|Y_{\tau e}|^2 + |Y_{e\tau}|^2} < 0.0020$, and $\sqrt{|Y_{\tau\mu}|^2 + |Y_{\mu\tau}|^2} < 0.0015$. Fig. 5 shows the limits on the individual coupling matrix elements $Y_{\tau\ell}$ and $Y_{\ell\tau}$ together with the limits from the ATLAS Run 1 analysis and from $\tau \to \ell\gamma$ searches [91,93].

9. Conclusions

Direct searches for the decays $H \to e\tau$ and $H \to \mu\tau$ are performed with proton–proton collisions recorded by the ATLAS detector at the LHC corresponding to an integrated luminosity of 36.1 fb^{-1} at a centre-of-mass energy of $\sqrt{s} = 13$ TeV. No significant excess is observed above the expected background from Standard Model processes. The observed (expected) upper limits at 95% confidence level on the branching ratios of $H \to e\tau$ and $H \to \mu\tau$ are 0.47% ($0.34^{+0.13}_{-0.10}$%) and 0.28% ($0.37^{+0.14}_{-0.10}$%), respectively. These limits are more stringent by a factor of 2 (5) than the corresponding limits for the $H \to e\tau$ ($H \to \mu\tau$) decay determined by ATLAS at $\sqrt{s} = 8$ TeV.

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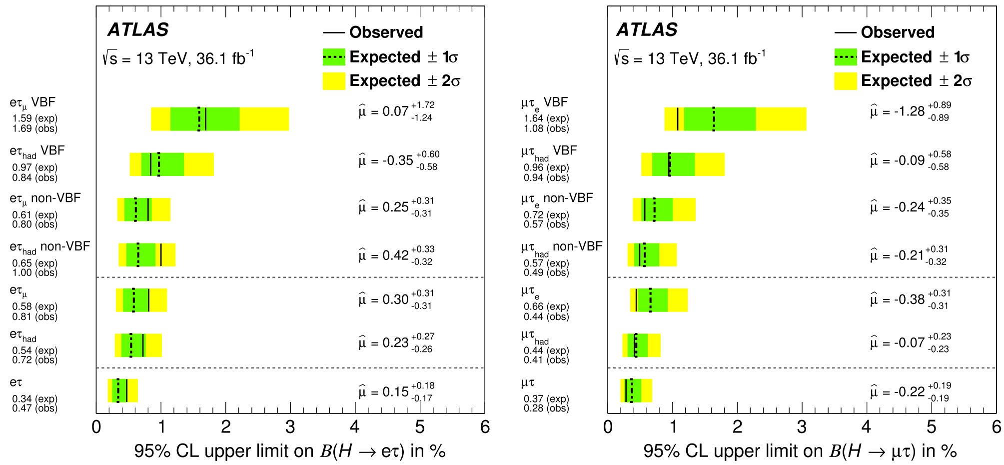

Fig. 4. Upper limits at 95% CL on the LFV branching ratios of the Higgs boson, $H \to e\tau$ (left) and $H \to \mu\tau$ (right), indicated by solid and dashed lines. Best-fit values of the branching ratios ($\hat{\mu}$) are also given, in %. The limits are computed while assuming that either $\mathcal{B}(H \to \mu\tau) = 0$ (left) or $\mathcal{B}(H \to e\tau) = 0$ (right). First, the results of the fits are shown, when only the data of an individual channel or of an individual category are used; in these cases the signal and control regions from all other channels/categories are removed from the fit. These results are finally compared with the full fit displayed in the last row.

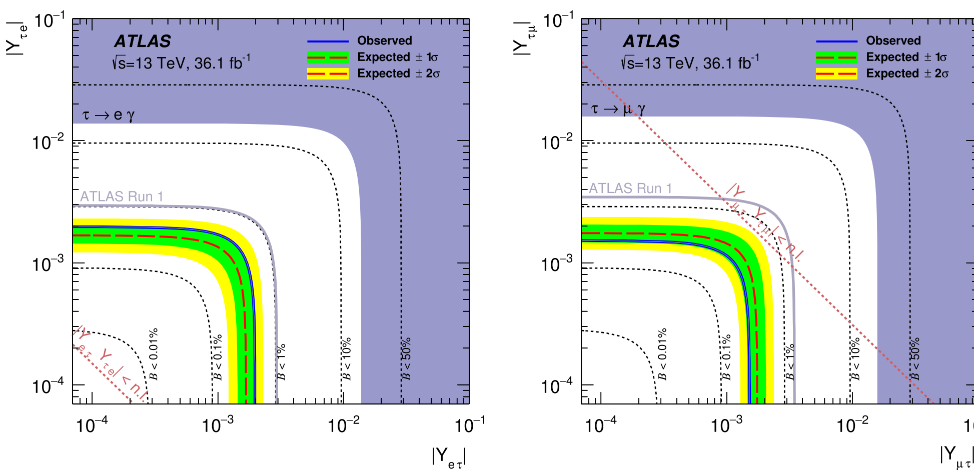

Fig. 5. Upper limits on the absolute value of the couplings $Y_{\tau\ell}$ and $Y_{\ell\tau}$ together with the limits from the ATLAS Run 1 analysis (light grey line) and the most stringent indirect limits from $\tau \to \ell\gamma$ searches (dark purple region). Also indicated are limits corresponding to different branching ratios (0.01%, 0.1%, 1%, 10% and 50%) and the naturalness limit (denoted n.l.) $|Y_{\tau\ell}Y_{\ell\tau}| \lesssim \frac{m_\tau m_\ell}{v^2}$ [91] where v is the vacuum expectation value of the Higgs field.

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